Practical Information

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First Principles Based Microkinetic Modelling of Methyl Butanoate Pyrolysis

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The increasing worldwide energy demand and reduced amount of petroleum reserves have created the need for sustainable development of alternatives. One of the possible alternatives is biodiesel, a fuel substitute produced from renewable resources such as vegetable oils or animal fats. Because of its complex composition, the direct modelling of biodiesel is difficult. First, an understanding of the reactivity of the oxygenated part of these molecules is required. Methyl butanoate (MB), CH3CH2CH2C(=O)OCH3, is a relatively short methyl ester that still incorporates all essential chemical structure features of a typical biofuel. It can therefore be used as a convenient model compound for the complex biofuel methyl ester mixture.

In this work, an ab initio based group additive model is built to describe the pyrolysis of methyl esters. The kinetic model is validated by comparison with a new set of experimental data gathered on a flow reactor. The experimental setup has been discussed in detail in previous work [1, 2]. For the pyrolysis of MB, the feed to the reactor is set to 257 g/h MB and 40 g/h N_2. The pressure is set to 0.17 MPa. In order to cover the complete conversion range, the temperature setting varies from 913 K to 1113 K in 20 K increments.

For the development of the microkinetic model for MB pyrolysis, the Genesys [3] software package for automatic kinetic model generation is used and adapted. The termination of the kinetic model generation is achieved with the rule-based criterion. For the determination of thermodynamics and kinetics of all compounds and reactions in the model, Genesys makes use of user-defined databases. These databases contain thermodynamic and kinetic data for hydrocarbon and oxygenated compounds that are calculated with CBS-QB3 composite method. If data is not available for certain compounds or reactions, estimation techniques are used. For thermodynamic data this includes Benson's group additivity method [4] and hydrogen increment method [5]. For rate coefficients, the group additivity method[6, 7] is used or analogy with reactions taken from literature data[8, 9].

The simulated MB conversion and major product yields agree well with experimental data acquired at the bench-scale setup over the studied temperature range. The majority of the major products are simulated within less than 10% relative deviation from the experimental values.

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